



chain nodes :

7 8 9 10 14 15 18 25 26 27 28 31 32 33 34 35

ring nodes :

1 2 3 4 5 6 19 20 21 22 23 24

ring/chain nodes :

11 12

chain bonds :

2-15 3-18 4-14 5-8 6-7 7-10 7-12 8-9 8-11 20-32 21-33 22-31 23-26 24-25 25-27
25-35 26-28 26-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 19-20 19-24 20-21 21-22 22-23 23-24

exact/norm bonds :

2-15 3-18 4-14 7-10 8-9 20-32 21-33 22-31

exact bonds :

5-8 6-7 7-12 8-11 23-26 24-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 19-20 19-24 20-21 21-22 22-23 23-24 25-27 25-35 26-28
26-34

G1:H,Ak,Ph

G2:X,Ak,Ph,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 14:CLASS 15:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom
25:CLASS 26:CLASS 27:CLASS 28:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS

fragments assigned reactant role:

containing 1